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N-(4-Methoxy-6-methyl-1,3,5-triazin-2-yl)-*N*-methyl-*N*′-(2,3,4-trifluorophenyl)urea

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.004 Å
R factor = 0.061
wR factor = 0.131
Data-to-parameter ratio = 13.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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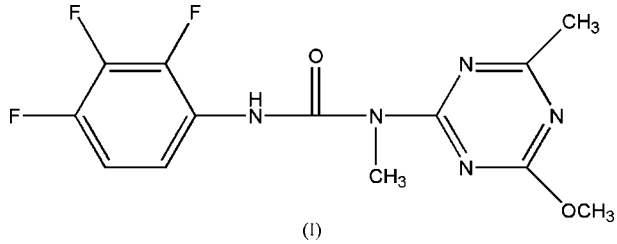
In the title compound, $C_{13}H_{12}F_3N_5O_2$, intramolecular N—H···F, N—H···N, C—H···O and C—H···N hydrogen bonds, and π–π stacking interactions generate a columnar structure along the *a* axis.

Comment

It is well known that substituted ureas containing a triazine group exhibit remarkable bioactivities such as herbicidal (Baumeister, *et al.*, 1994), plant-growth regulatory (Douglass & Moon, 1987), antitubercular (Patel, *et al.*, 2003) and antibacterial activity against *Staphylococcus aureus* and *Escherichia coli* (Patel, *et al.*, 2003). We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1 and selected bond lengths and angles are given in Table 1. The dihedral angle between the planes of the 1,3,5-triazine and trifluorophenyl fragments is 10.1 (2)°. Four intramolecular hydrogen bonds, N—H···F, N—H···N, C—H···O and C—H···N (Desiraju & Steiner, 1999), are observed in the molecule (Table 2, Fig. 1). In the crystal structure, the molecules are stacked along the *a* axis, forming a columnar structure (Fig. 2). In the column, the interplanar distance of 3.35 (9) Å between benzene rings suggests π–π stacking interactions; this is shorter than the π-cloud thickness (3.42 Å; Pauling, 1960).

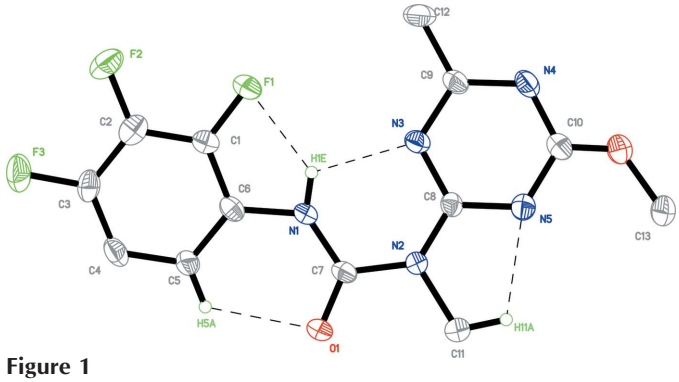


Figure 1
The molecular structure of (I), drawn with 30% probability ellipsoids. Intramolecular hydrogen bonds are indicated by dashed lines.

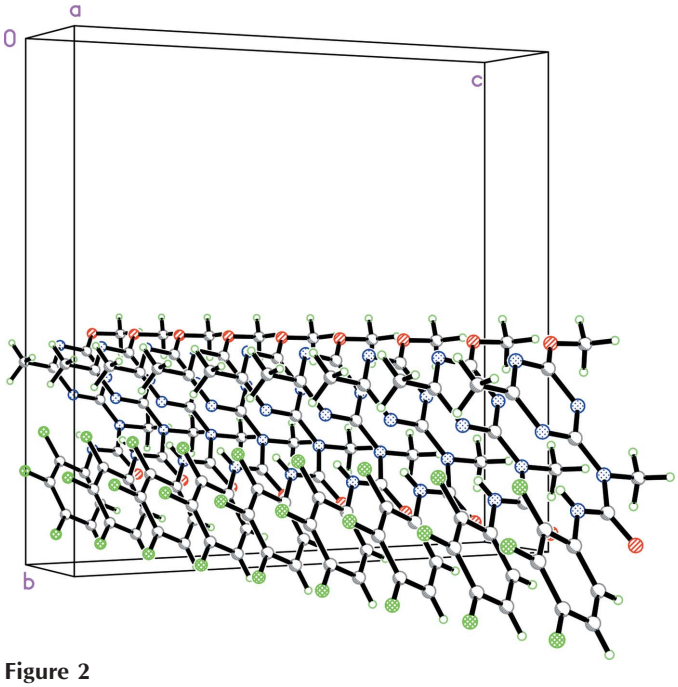


Figure 2
A packing diagram for (I), with a pronounced column along the *a* axis realised by π–π stacking.

Experimental

4-Methoxy-*N*,6-dimethyl-1,3,5-triazin-2-amine (1.54 g, 10 mmol) was added to an anhydrous acetonitrile solution of 2,3,4-trifluorophenyl isocyanate (1.91 g, 10 mmol), and the mixture was stirred at 333 K for 3 h under nitrogen. A colourless precipitate was isolated, recrystallized from ethyl acetate–hexane mixture (3: 1 *v*/*v*) and dried *in vacuo* to give a pure compound in 86.2% yield. Colourless needle-like single crystals (m.p. 425–426 K) suitable for X-ray analysis were obtained by slow evaporation of a methanol solution. Analysis calculated for $C_{13}H_{12}F_3N_5O_2$: C47.71%, H3.70%, N21.40%; found: C47.74, H3.68, N21.45%.

Crystal data

$C_{13}H_{12}F_3N_5O_2$
M_r = 327.28
Monoclinic, $P2_1/c$
a = 4.4215 (9) Å
b = 17.836 (4) Å
c = 18.337 (4) Å
β = 91.55 (3)°
V = 1445.6 (5) Å^3
Z = 4
D_x = 1.504 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 764 reflections
θ = 2.0–14.1°
μ = 0.13 mm^{-1}
T = 291 (2) K
Needle, colourless
0.20 × 0.18 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.97, T_{max} = 0.98
7065 measured reflections
2853 independent reflections
2004 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 26.0°
$h = -5 \rightarrow 5$
$k = -21 \rightarrow 22$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.131
S = 1.01
2853 reflections
215 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.66P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—F1	1.324 (3)	C8—N3	1.385 (3)
C2—F2	1.350 (3)	C9—N3	1.380 (3)
C3—F3	1.349 (3)	C9—N4	1.384 (3)
C6—N1	1.427 (3)	C10—O2	1.158 (3)
C7—O1	1.213 (3)	C10—N4	1.368 (4)
C7—N1	1.350 (3)	C10—N5	1.369 (3)
C7—N2	1.408 (3)	C11—N2	1.503 (3)
C8—N2	1.320 (3)	C13—O2	1.438 (4)
C8—N5	1.381 (3)		
O1—C7—N1	123.5 (2)	C8—N2—C7	128.1 (2)
O1—C7—N2	120.0 (2)	C8—N2—C11	117.5 (2)
N4—C9—C12	120.0 (2)	C7—N2—C11	114.4 (2)
C7—N1—C6	127.4 (2)	C10—O2—C13	126.1 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*E*···F1	0.81 (4)	2.05 (4)	2.687 (3)	135 (3)
N1—H1*E*···N3	0.81 (4)	2.14 (4)	2.575 (3)	114 (3)
C5—H5*A*···O1	0.93	2.29	2.872 (3)	120
C11—H11*A*···N5	0.96	2.19	2.688 (4)	111

All H atoms were placed in calculated positions and were refined isotropically, with U_{iso}(H) values constrained to 1.2U_{eq}(C, N), using a riding model, with C—H = 0.93–0.96 Å and N—H = 0.82 Å.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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